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# MODEL PREDICTIVE CONTROL OF LARGE-SCALE SYSTEMS: APPLICATION TO THE TENNESSEE EASTMAN PROCESS

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## Abstract

Highly nonlinear and open-loop unstable processes pose serious difficulties to the implementation of optimal control solutions, such as Model Predictive Control (MPC). An example of such processes is the Tennessee Eastman model. Here we show that by proper combination of the optimization algorithm with additional intermediate layers of control, most of the ill-conditioning can be avoided, without loss of performance. Simulation results of our control strategy are compared with previously published results. The numerical efficiency of the solution procedure is addressed, and some characteristics of the problem that can be further exploited are also identified.

## 1 Introduction

The real-world application of advanced supervision strategies for process control, such as Nonlinear Model Predictive Control (NMPC), is often limited by a number of factors such as the size of the numerical problems that need to be solved, or difficulties in handling highly nonlinear and open-loop unstable models. These characteristics are commonly found in a large number of chemical processes. In both situations, the numerical difficulties that arise in the solution of these problems can lead to an important degradation of the control performance or even failure of the optimization algorithms, in more extreme situations. These limitations need to be addressed in an efficient manner in order to make a wider online application of NMPC possible.

This paper discusses the difficulties in the application of NMPC to a complex process model, the Tennessee Eastman benchmark. A short description of this model is given next, followed by the presentation of some results obtained in a previous detailed dynamic analysis of this model [4].

## 2 The Tennessee Eastman Benchmark

The Tennessee Eastman (TE) problem, presented by [2], involves a highly nonlinear open-loop unstable process composed of a reactor/separator/recycle arrangement in a total of five operation units. Two liquid products are obtained through a network of four exothermic, irreversible reactions:

$$A_{(g)} + C_{(g)} + D_{(g)} \longrightarrow G_{(l)} \quad (1)$$

$$A_{(g)} + C_{(g)} + E_{(g)} \longrightarrow H_{(l)} \quad (2)$$

$$A_{(g)} + F_{(g)} \longrightarrow F_{(l)} \quad (3)$$

$$3D_{(g)} \longrightarrow 2F_{(l)} \quad (4)$$

A total of eight chemical species are involved. The original process model comprises fifty state variables, forty one measured variables and twelve variables available for manipulation. Within the measured variables, twenty one are gas and liquid compositions, all subject to delays. A diagram of the process is shown in Figure 1.

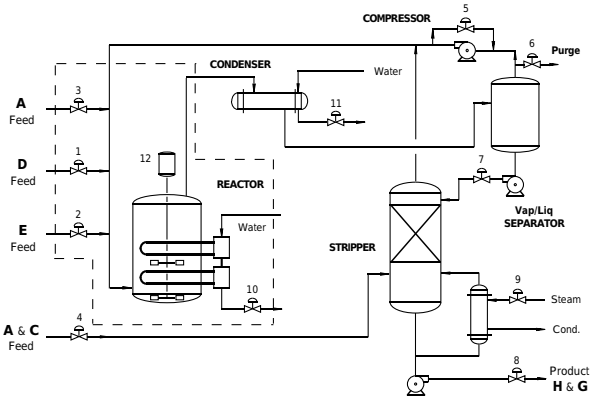


Figure 1: The Tennessee Eastman process.

Due to its realistic complexity, the TE problem is an excellent benchmark to test and compare the applicability of control solutions to industrial problems. Various solutions have been proposed, ranging from SISO multi-loop strategies to NMPC. Among the SISO multi-loop control strategies the ones in [6] and [12] stand out. In [12] a decentralized control structure, using only of PI controllers, is proposed. In the design procedure used, a method for production rate control was initially selected, to which all other control functions are then coordinated. An interesting aspect of this structure is that all flow rates depend on the production rate through a complex ratio control. The results presented in [6] are surprising, since only proportional controllers are used. This is achieved by selecting



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and tuning the controllers using a predefined hierarchy, again beginning with the production rate. This structure explicitly takes into account the instability of the reactor, which is treated as an additional constraint in the sense that reactor temperature control is required. A common aspect between these two structures is the need for override controllers to deal with specific situations, such as the signal change of the steady-state gain of some output variables with respect to the input variables. A review of other proposed solutions can be found in [5].

## 3 The Tennessee Eastman Reactor

Early work with the TE process showed that the unit with the most significant contribution to the overall instability of the process was the reactor. In order to better understand its characteristics, a model of the reactor was isolated from the original process model, corresponding to the zone inside the dashed line in Figure 1. Using this model, we studied the reactor open-loop response, the sensitivity of the output variables with respect to the input variables and computed the eigenvalues of the corresponding linearized model [4].

With all of the disturbances tested, the reactor quickly reached its shutdown limits, sometimes in less than an hour. We could also observe significant inverse response behavior, due to the competition between the reaction and the vaporization phenomena taking place simultaneously in the reactor.

A sensitivity analysis was performed, computing a new steady state for every different value of a given manipulated variable, while keeping the remaining ones at their nominal values. The results obtained can be plotted similarly to Figure 2, in this case for variations of the reactor level, pressure and temperature with the reactor cooling water flow.

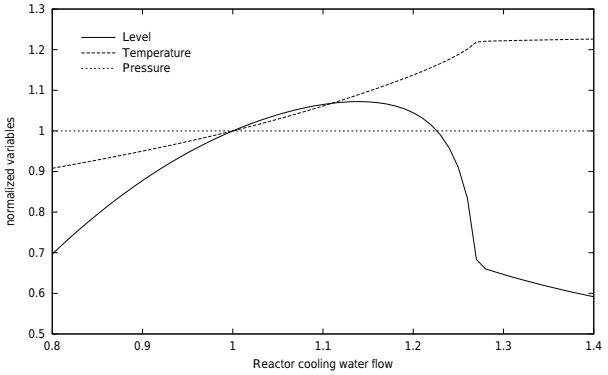


Figure 2: Sensitivities of the reactor output variables versus reactor cooling water flow (all variables are normalized).

The slope of each curve can be interpreted as the steady-state gain of the variable at that point. In Figure 2 we can see that the steady-state gain of the reactor level with respect to the cooling water flow changes sign in the vicinity of the original steady state. This introduces difficulties in the use of fixed linear controllers, especially in the region where the gains of the output variables change.

By linearization, using numerical derivatives, we were able to obtain a model for the reactor in the form

$$\dot{x} = Ax + Bu \tag{5}$$
$$y = Cx, \tag{6}$$

using deviation variables, with $x \in \mathbf{R}^{n_s}$, $u \in \mathbf{R}^{n_i}$, and $y \in \mathbf{R}^{n_o}$. An inspection of the eigenvalues of the state matrix confirms the strict open-loop instability of the reactor. All eigenvalues are real, ranging from $-720\,\mathrm{h}^{-1}$ to $12.2\,\mathrm{h}^{-1}$. The wide range of the magnitudes of the eigenvalues indicates different time scales of variation within the reactor. The results presented in this section clearly indicate that much better reactor control is to be expected from nonlinear strategies over linear controllers alone.

## 4 Nonlinear MPC Algorithm

The Model Predictive Control formulation used in this work assumes a process model of the form

$$\dot{x} = f(x, u, d; \theta) \tag{7}$$
$$y = g(x; \theta), \tag{8}$$

where $f$ and $g$ are twice continuously differentiable functions, and $x \in \mathbf{R}^{n_s}$ is the state vector, $u \in \mathbf{R}^{n_i}$ is the input vector and $y \in \mathbf{R}^{n_o}$ is the output vector. Perfect knowledge of the state variables is assumed. By taking the linearization of the model equations around a nominal control trajectory, $\bar{U}$, it is possible to obtain the solution of the nonlinear control problem through the use of an SQP-type method. The quadratic problem solved at each iteration of this method is of the form

$$\min_{\Delta U} \quad J_2 = (E - \mathcal{S}_m \Delta U)^{\mathrm{T}} Q_1 (E - \mathcal{S}_m \Delta U) + (\Delta U - U')^{\mathrm{T}} Q_2 (\Delta U - U') \tag{9}$$
$$\text{s.t.} \quad U_{ld} \leq \Delta U \leq U_{ud}, \tag{10}$$
$$Y_{ld} \leq \mathcal{S}_m \Delta U \leq Y_{ud}, \tag{11}$$

where $E = Y_{\mathrm{sp}} - \bar{Y}$, $U' = U_r - \bar{U}$, $\Delta U = U - \bar{U}$, $Y_{sp}$ is the set-point vector, $\bar{Y}$ is the output trajectory obtained by using $\bar{U}$, $Q_1$ and $Q_2$ contain the penalties for the deviations of the outputs and inputs from their reference trajectories. $\mathcal{S}_m$ is the dynamic matrix, obtained by the linearization of the model equations. Details on this algorithm can be found in [11].

## 5 Compensator Design

Due to the highly nonlinear and open-loop unstable nature of the TE reactor, the MPC formulation is not able, by itself, to deal efficiently with the problem [13, 14]. This is mainly due to failures in the ODE solver and to the severe ill-conditioning of the optimization problem. To overcome these difficulties we consider the presence of an inner compensator, located between the process and the MPC level, as shown in Figure 3. The purpose of this extra layer of control is to avoid, as much

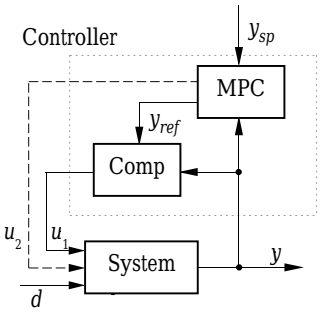


Figure 3: Location of the inner compensator.

as possible, the open-loop instability and the consequent ill-conditioning introduced in the optimization formulation.

To design the inner compensator we started by considering the use of simple linear SISO loops. For this purpose, we considered all possible pairings between the output variables and the control variables, with a proportional controller. The most adequate pairing is selected by analyzing the variation of the largest eigenvalue of the closed-loop state matrix state matrix

$$\lambda_{\max} = \max_{1 \le i \le n_s} \{\lambda_i(A + B\ K_p\ C)\}$$

with the proportional controller gain, $K_p$. Of the forty possible pairings only six are feasible, i.e., capable of stabilizing the reactor. Further selection between the feasible pairings was made by implementing them individually in continuous time, and testing all the input disturbances proposed by [2] that affect the reactor. The pairing for which better results were obtained was the one between the reactor temperature and the reactor cooling water flow. Since this loop was able, by itself, of stabilizing the reactor, it was selected for use as the inner compensator with $K_p = 25$ (using normalized variables). In this control configuration the set-point of the compensator is a decision variable in the control problem, thus no degrees of freedom are lost. Simulation results with NMPC and this compensator applied to the reactor model showed that good dynamic behavior could be obtained, without significant ill-conditioning [4].

## 6 Process Control Results

When using the MPC algorithm to control the entire TE process we observed similar problems to those that occurred when controlling the reactor alone. Since the reactor is the main source of instability, we decided to reevaluate the same compensator with the entire process, instead of repeating the selection algorithm. This proved to be a good choice since both the ill-conditioning and the numerical instability in the solution of the model equations were still avoided.

Figure 4 shows the profiles of the most important process variables, for a product mix change at time $t = 1$ hour, in the presence of a slow random drift in the reaction kinetics (set-point change 2 and disturbance `IDV(13)` in [2]). Normalized values are used in all curves. The variables whose set-points are changed are the compositions in the final product of $G$ (decreased by 18%) and H (increased by 22%).

The tuning parameters used are $Q_u = 1$ (for all the inputs), $Q_y = 1$ for the product flow-rate, $G$ and $H$ compositions and all of the measured byproduct compositions. For the remaining measured variables a value of $Q_y = 0$ was used, since a new set-point wasn't available for them. The predictive horizons comprise $m = 4$ and $p = 8$ sampling intervals, for manipulation and prediction, respectively. The sampling interval used was $T = 0.1$ hours. Integral action is applied to $G$ composition, with a gain of 10 $h^{-1}$.

In Figure 4(g) we can see that the set-point change is accomplished in less than 1 hour, and the variables remain thereafter within an interval of $\pm 0.5\%$ of the desired values. This is a remarkable result, given that during the disturbance the deviation between the process and model kinetics can reach up to 20%. Although this is not a realistic situation, it is a good test of the controller performance and robustness.

In Figure 4(a) we can see that the new set-point is in part achieved through changes in the relative quantities of reactants $D$ and $E$ entering the process, as would be expected from reactions (1) and (2). Also important is the decrease of the reactor level (Figure 4(c)), since this causes an increase of the residence time of the gaseous reactants in the reactor. In the starting conditions, the data of [2] show that reaction (1) is almost complete, while the amount of $H$ produced is only a fraction of what would be obtained if reaction (2) was complete. Thus an increase in the residence time is favorable to a higher production of $H$.

As the reactor level decreases there is a need to store the material that abandons it, in order to keep the product flow rate approximately constant. This is achieved through an increase in the separator and stripper levels, the only units with storage capacity. As we can observe in Figures 4(d) and 4(f) these levels increase up to their upper limits.

Since all the reaction rates depend on the partial pressures of the involved reactants, a decrease in these (caused by the increase of the gas volume in the reactor) would have undesirable effects on the production rate. To avoid this the controller increases the reactor pressure close to its upper limit (Figure 4(c)) thus counterbalancing the effect of the level decrease. The increase of the separator and stripper pressure is a consequence of the rise in the reactor pressure.

The product composition change could be more easily achieved at higher reactor temperatures, due to higher selectivity. But, as we can see in Figure 4(h), the controller keeps the reactor temperature set-point near its initial value for most of the time. This is due to the need of avoiding excessive byproduct $F$ formation, favored by higher temperatures. Since the byproduct only leaves the process through the purge, which has a small flow rate, an increase in its production would cause an excessive accumulation in the process and a potential uncontrolled rise in the pressure of all units, thus making the process harder to control.

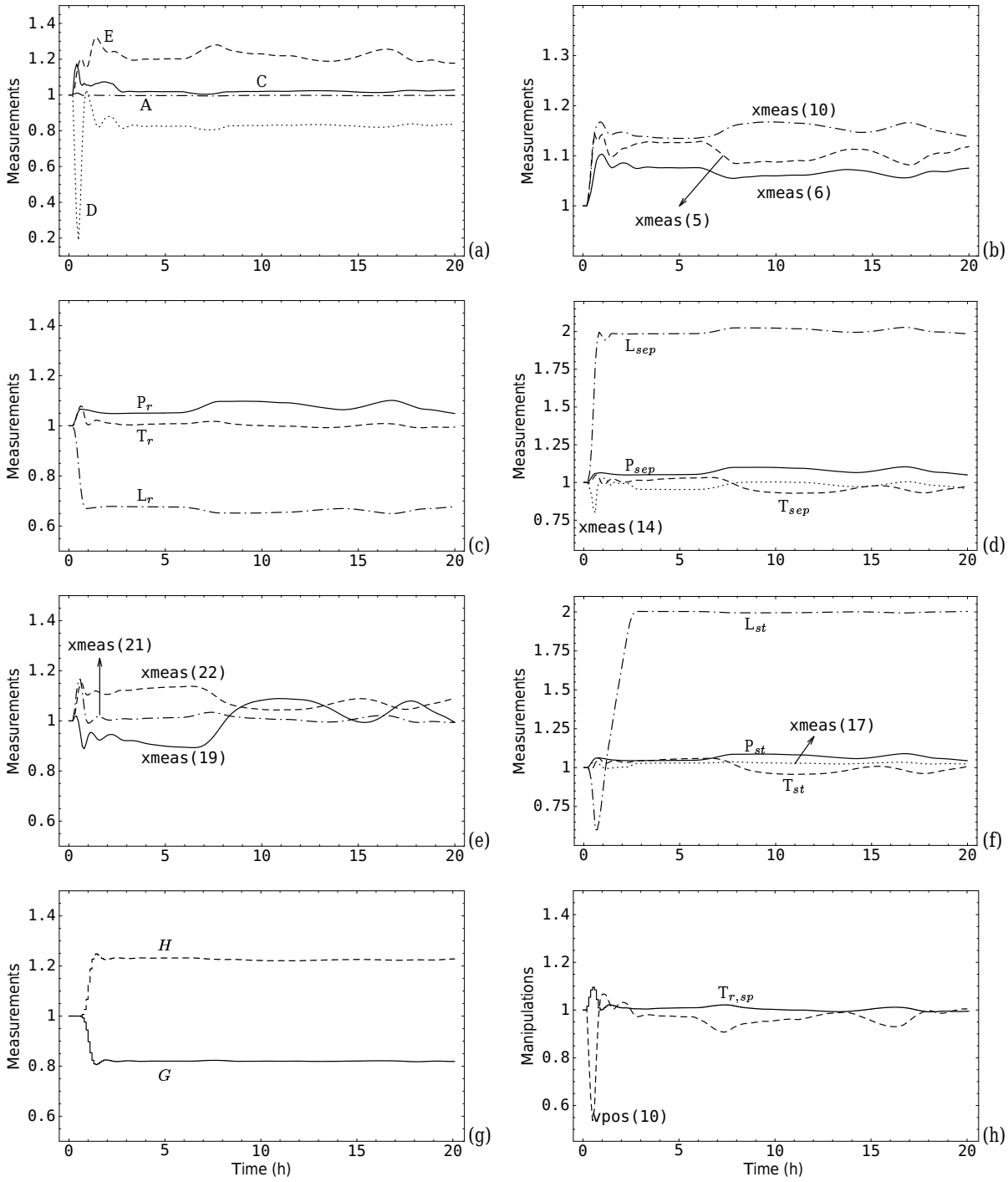


Figure 4: Closed loop response to a set-point change in the product composition, at time $t = 1$ h, in the presence of a slow drift in the reaction kinetics. (a) feed flows; (b) `xmeas(5)` - recycle flow, `xmeas(6)` reactor feed rate, `xmeas(10)` purge rate; (c) reactor pressure, level and temperature; (d) separator pressure, level and temperature, `xmeas(14)` - separator underflow; (e) `xmeas(19)` - stripper steam flow, `xmeas(21)` - reactor cooling water outlet temperature, `xmeas(22)` - separator cooling water outlet temperature; (f) stripper pressure, level and temperature, `xmeas(17)` stripper underflow (product); (g) $G$ and $H$ compositions in the product; (h) $T_{r,sp}$ - reactor temperature set-point, `vpos(10)` - reactor cooling water valve position.

The results presented were obtained with a tolerance of $5 \times 10^{-4}$ for the convergence of the control profiles. The state variables were computed with absolute and relative tolerances of $0.5 \times 10^{-7}$. The model sensitivities, needed by the control algorithm, were computed with absolute and relative tolerances of $2.5 \times 10^{-7}$.

The maximum number of iterations of the control algorithm was 8, in the sampling interval where the set-point change and active constraints are firstly detected. This control structure, with the control parameters presented, is able to efficiently change the product composition, even in the presence of significant deviation between the process and the model used by the MPC. All of the control objectives required by [2] are met, even though four output variables are at their upper operating limits during most of the simulation. For comparison the same set-point, in the absence of disturbances, is accomplished in 4, 7 and 10 hours by the SISO multi-loop control structures proposed by [6], [12] and [7], respectively.

The changes in the numerical conditioning of the optimization problem caused by the introduction of the compensator are shown in Table 1. As can be observed, the Hessian matrix of the quadratic problem is extremely ill-conditioned when using MPC only. A significant reduction of this ill-conditioning, for the same tuning parameters, is achieved by the introduction of the compensator, thus making the control problem easier to handle. This has the desired effect of reducing the number of iterations needed for convergence of the control profiles.

| | MPC | MPC + compensator |
|---|---|---|
| Reactor | $4.6 \times 10^6$ | 2.3 |
| Process | $5.6 \times 10^5$ | 210 |

Table 1: Hessian matrix condition for the different control configurations.

## 7 Improving the numerical efficiency of the solution

In this section we analyze the numerical performance of the computational package used to obtain these results. This package, written for the development of MPC algorithms [10], is divided in three main modules. Each module is typically executed as an independent process in a UNIX workstation. The NEWCON module implements the NMPC algorithm, the QP module solves the quadratic optimization subproblems, while the INTEG module integrates the model and sensitivity equations.

An analysis of the CPU time spent in the routines of each module led to the conclusion that the most computationally expensive procedure in the algorithm is the computation of the model sensitivities, taking approximately 47% of the total CPU time. Initially this was done by DDASAC [1], which implements a staggered direct method where the linear sensitivity equations are solved directly only after convergence of the state variables. This requires the computation and factorization of the Jacobian at each step, which is clearly not an attractive feature when dealing with systems of considerable dimension such as the TE. In view of this, a different approach for the solution of the sensitivities equations was necessary, in order to improve its numerical efficiency. From the available alternatives, we selected the staggered corrector and simultaneous corrector methods [3, 9]. The first method is similar to the staggered direct approach, but the sensitivity linear system is solved by a Newton iteration, where the factored Jacobian matrix is the one used for the solution of the state equations. In the simultaneous corrector method the state and sensitivity equations are solved as one linear system, using a block diagonal approximation of the full Jacobian. Both of these methods are implemented in the DDASPK3.0 routines [8], which we used to replace DDASAC in the INTEG module.

In Table 2 we present the total CPU time and the percentage spent in the INTEG module for its different configurations, corresponding to the first two hours of the simulation results presented in Figure 4.

| | DDASAC | DDASPK |
|---|---|---|
| Total CPU time (sec) | 2322.023 | 1560.547 |
| Sensitivities time (%) | 47 | 28 |

Table 2: Total CPU time and percentage spent in solving the sensitivity equations for different INTEG modules.

As can be observed a significant decrease in the CPU time can be obtained through the use of the simultaneous corrector method, implemented in DDASPK. Also the solution of the sensitivity equations is done in a more efficient manner. The CPU time decrease is mostly due to the fewer number of Jacobian evaluations and, thus, to the fewer times dense matrixes need to be factorized. Figure 5 shows that, for an absolute tolerance of $0.5 \times 10^{-7}$, with which all the results presented above were obtained, the number of Jacobian computations needed by DDASAC is about eight times the one needed by DDASPK.

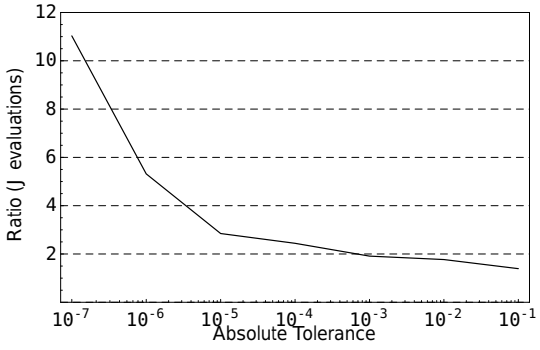


Figure 5: Ratio between the Jacobian evaluations needed by DDASPK and by DDASAC, versus the logarithm of the absolute tolerance for the sensitivity computation.

The CPU time profiles obtained for simulations using DDASPK show that about 35% of the time is still spent in the linear algebra routines (such as BLAS), showing that there is still room for improvement in the efficiency of the solution of the linear systems involved. No significant differences have been found, for this problem, between the simultaneous and staggered corrector methods. The numbers presented are representative of all of the simulations carried so far.

These results show that the limiting step in the algorithm is the direct solution, through factorization, of the linear problems. Further improvements can be accomplished by exploiting the structure of the Jacobian matrix of the TE process. Even though this is an unsymmetric matrix with a large fill, the lines and columns corresponding to the dynamics of the valves have few non-zeros elements outside the diagonal and a fixed structure. This property can be used to reduce the dimension of the linear systems to be solved. The possibility of using iterative methods to solve the linear equations can also be taken into account, even though this requires the selection of a preconditioner, a non-trivial task in the case of the TE. This is the subject of current investigation.

## 8 Conclusions

In terms of control performance, the simulation results presented for the TE process, obtained using NMPC with an inner compensator, compare very favorably with other previous results for this process. The control structure is able to handle well output gain changes, tight constraints and open-loop instability. In terms of numerical performance, these simulations allowed also the identification of the limiting steps, such as the sensitivity computation. A different method was tested and significant improvements were achieved. Further improvements are still possible through the use of more efficient algorithms to solve large systems of linear equations.

## Acknowledgments

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